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Abstract

The main results of our research related to first passage time (FPT) problems for stationary Gaussian processes are synthetically outlined. The vectorized and parallel algorithm, efficiently implemented on CRAY-T3E in FORTRAN90-MPI, allows to simulate a large number of sample paths of Gaussian stochastic processes in order to obtain reliable estimates of probability density functions (pdf) of first passage times through pre-assigned boundaries. The class of Gaussian processes characterized by damped oscillatory covariance functions and by Butterworth-type covariances have been extensively analyzed in the presence of constant and/or periodic boundaries. The analysis based on our simulation procedure has been particularly profitable as it has proved to provide an efficient research tool in all cases of interest to us when closed-form results or analytic evaluations were not available. Last but not least, in some cases it has allowed us to conjecture certain general features of FPT densities that successively have been rigorously proved.

Si illustrano sinteticamente gli sviluppi della nostra ricerca in merito al problema del tempo di primo passaggio per processi gaussiani stazionari. L'algoritmo vettoriale e parallelo, efficentemente implementato sul CRAY-T3E in FORTRAN90 e in ambiente MPI, ha reso possibile simulare un elevato numero di realizzazioni di processi stocastici gaussiani fino a poter disporre di affidabili stime delle densità del tempo di primo passaggio. Le classi di processi gaussiani con funzione di covarianza ad oscillazioni smorzate e con funzione di covarianza di tipo Butterworth sono state estensivamente analizzate in presenza di barriere costanti e/o periodiche. Lo studio basato sulle simulazioni si è così rivelato particolarmente utile anche perché ha costituito uno strumento di indagine efficiente in tutti quei casi nei quali soluzioni in forma chiusa sono risultate inaccessibili o gli strumenti analitici inadeguati; inoltre, talora ha lasciato intuire nuove congetture la cui validità è poi stata rigorosamente dimostrata.

1 The FPT problem

The first passage time (FPT) problem involves the determination of the probability distribution function of the random variable T representing the instant when for the first time a dynamic system, modeled by a stochastic process, enters a pre-assigned critical region of the state space. Numerous examples stressing the relevance of FPT problems are offered by various fields: in theoretical neurobiology the neuronal firing may sometimes be viewed as a FPT of the potential difference across the neuronal membrane through some threshold value; in astrophysics one can think of the time necessary for a star to escape from a galaxy; other examples are offered by fields as diversified as economy or psychology and, of course, mechanical engineering in which first passage time problems bear relevance in the context of stability and integrity of systems subject to random vibrations (cf, for instance, [6]).

In the neurobiological context a classical approach to model FPT problems consists of invoking diffusion processes as responsible for the fluctuations of the stochastic system under the assumption of numerous simultaneously and independently acting input processes (see [8] and references therein). All these models rest on the strong Markov assumption, which implies the possibility of making use of various analytic methods for the FPT pdf evaluation. However, it is conceivable that, particularly if the described system is subject to strongly correlated inputs, the Markov assumption is inappropriate, so that models based on non-Markov stochastic processes ought to be considered. By analogy with Gernstein-Mandelbrot and Ornstein-Uhlenbeck models ([8]), one can thus challenge the use of correlated Gaussian processes. However, the difficulty stems out of the lack of effective analytical methods for obtaining manageable closed-form expressions for the FPT probability density. Indeed, let $\{X(t), t \geq 0\}$ be a one-dimensional non-singular stationary Gaussian process with mean $E[X(t)] = 0$ and covariance $E[X(t)X(\tau)] = \gamma(t-\tau) = \gamma(\tau-t)$ such that $\gamma(0) = 1, \dot{\gamma}(0) = 0$ and $\ddot{\gamma}(0) < 0$. Furthermore, let $S(t) \in C^1[0,\infty)$ be the threshold, with $S(0) > x_0$. The FPT random variable is defined as follows:

$$T = \inf_{t \geq 0}\{t : X(t) > S(t)\} \qquad \text{with } X(0) = x_0,$$

and the FPT probability density function $\frac{\partial P(T \leq t)}{\partial t} \equiv g[S(t), t|x_0]$ of $X(t)$ through $S(t)$, is given by ([9])

$$g[S(t), t|x_0] = W_1(t|x_0) + \sum_{i=1}^{\infty}(-1)^i \int_0^t dt_1 \int_{t_1}^t dt_2 \cdots \int_{t_{i-1}}^t dt_i W_{i+1}(t_1, \ldots, t_i, t|x_0), \tag{1}$$

with

$$W_n(t_1, \ldots, t_n|x_0) = \tag{2}$$
$$\int_{\dot{S}(t_1)}^{\infty} dz_1 \cdots \int_{\dot{S}(t_n)}^{\infty} dz_n \prod_{i=1}^{n} [z_i - \dot{S}(t_i)]\, p_{2n}[S(t_1), \ldots, S(t_n); z_1, \ldots, z_n|x_0],$$

where $p_{2n}(x_1, \ldots, x_n; z_1, \ldots, z_n | x_0)$ is the joint pdf of $X(t_1), \ldots, X(t_n), Z(t_1) = \dot{X}(t_1), \ldots, Z(t_n) = \dot{X}(t_n)$ conditional upon $X(0) = x_0$.

The computational complexity of the above equations indicates that alternative procedures should be used in order to obtain information on the FPT distribution functions.

A simulation procedure, in details described in [3], has been implemented in order to disclose the essential features of the FPT densities for a class of Gaussian processes and specified boundaries. Our approach relies on a simulation procedure by which sample paths of the stochastic process are constructed and their first crossing instants through assigned boundaries are recorded. The underlying idea can be applied to any Gaussian process having spectral densities of a rational type. Since the sample paths of the simulated process are generated independently of one another, the simulation procedure is particularly suited for implementation on vector and supercomputers.

1.1 Butterworth covariance function

Extensive computations have been performed by us to explore the possible different shapes of the FPT densities as induced by the oscillatory behaviors of covariances and thresholds. In [3] we refer to the $\{X(t), t \geq 0\}$ stationary, zero-mean normal process with the oscillatory covariance

$$\gamma(t) := E[X(t+\tau)X(\tau)] \equiv \sqrt{2}\, e^{-\alpha\, t} \sin(\alpha\, t + \pi/4) \quad t \geq 0, \quad \alpha \in R^+, \quad (3)$$

known as Butterworth-type covariance, which is the simplest type of covariance carrying a concrete engineering significance ([10]). We consider separately the case of the varying boundary of the form

$$S(t) = S_0 + A \sin(2\pi t/Q)\,, \text{ (initially increasing)}, \quad (4)$$

and that of the varying boundary of the form

$$S(t) = S_0 + A \cos(2\pi t/Q)\,, \text{ (initially decreasing)},$$

where S_0, A and Q are positive constants. Such investigations have led us to formulate conjectures on the influence of the ratio $\frac{Q}{P}$, where Q is the threshold period and P is the covariance period, on the behaviour of $g[S(t), t|x_0]$. In addition, we gave numerical evaluation of $W_1(t|x_0)$, the first term in the right hand of (1), which we used to validate the reliability of estimates obtained by simulations in correspondence of small values of time t.

1.2 Damped oscillatory covariance function and double boundary case

Motivated by their relevance for numerous applications, we have implemented the simulation procedure for stationary normal processes $\{X(t), t \geq 0\}$ characterized by a more general damped oscillatory covariance function depending on two parameters ([5])

$$\gamma(t) \equiv \exp(-\beta t)\cos(\alpha t), \text{ with } t \geq 0, \quad \alpha, \beta \in \mathbf{R}^+, \quad (5)$$

and we estimated first passage time densities, conditional upon $X(0) = x_0$, through pairs of smooth boundaries, a constant and a periodic one:

$$\begin{cases} \theta_1(t) &= -A, \\ \theta_2(t) &= A + \sin\left(\dfrac{2\pi t}{Q}\right), \end{cases} \qquad t \geq 0,\ A, Q \in \mathbf{R}^+. \tag{6}$$

The results of some simulations are shown and conclusions are drawn on the effects of the periodic components of covariances and boundaries on qualitative and quantitative features of the following first passage time densities

$$g^+(t|x_0) := \frac{\partial}{\partial t} P\left\{\inf_{t\geq 0}\left[t : X(t) > \theta_2(t); X(\tau) > \theta_1(t), \forall \tau \in (0,t)\right]\right\}, \tag{7}$$

denoting the FPT density through the upper boundary,

$$g^-(t|x_0) := \frac{\partial}{\partial t} P\left\{\inf_{t\geq 0}\left[t : X(t) < \theta_1(t); X(\tau) < \theta_2(t), \forall \tau \in (0,t)\right]\right\}, \tag{8}$$

denoting the FPT density through the lower boundary, $g\,(t|x_0) = g^+\,(t|x_0) + g^-\,(t|x_0)$, denoting the FPT density of $X(t)$ through either boundaries and, finally, the $g_s\,(t|x_0)$ providing the FPT density of $X(t)$ through only one boundary of that in (6) (see Fig.1).

2 The upcrossing FPT problem

The upcrossing first passage time problem through varying boundaries, in which the $X(0)$ does not possess a delta-type probability density function, is considered. At first, focusing the attention on the problem of single neuron's activity modeling, we have considered some earlier contributions by A.I. Kostyukov *et al.* ([7]) in which a non-Markov process of a Gaussian type is assumed to describe the time course of the neural membrane potential. After re-formulating the problem in a rigorous framework, defining the upcrossing FPT density $g_u[S(t), t]$, and pinpointing the limits of validity of the model we compared in [4] Kostyukov's results on the firing probability density with those obtained by us by means of an ad hoc numerical algorithm implemented for the leaky integrator diffusion firing model with a variety of data constructed by the simulation procedure of non-Markov Gaussian processes with pre-assigned covariances. As shown in Fig.2, for different values of correlation time $\theta := \int_0^\infty |\gamma\,(\tau)|\, d\tau$, the parallel procedure allowed us to simulate the behavior of a class of Gaussian processes with covariance (5) in the presence of decreasing boundary $S(t) = 5 - t$. See [4] for details.

Along the lines indicated in [9], we have provided a series expansion of the upcrossing probability density function of the first passage time. Specifically, along the paradigm of a more extensive analysis of Gauss-Markov processes ([1]), we introduced, in corrispondence of a fixed real number $\varepsilon > 0$,

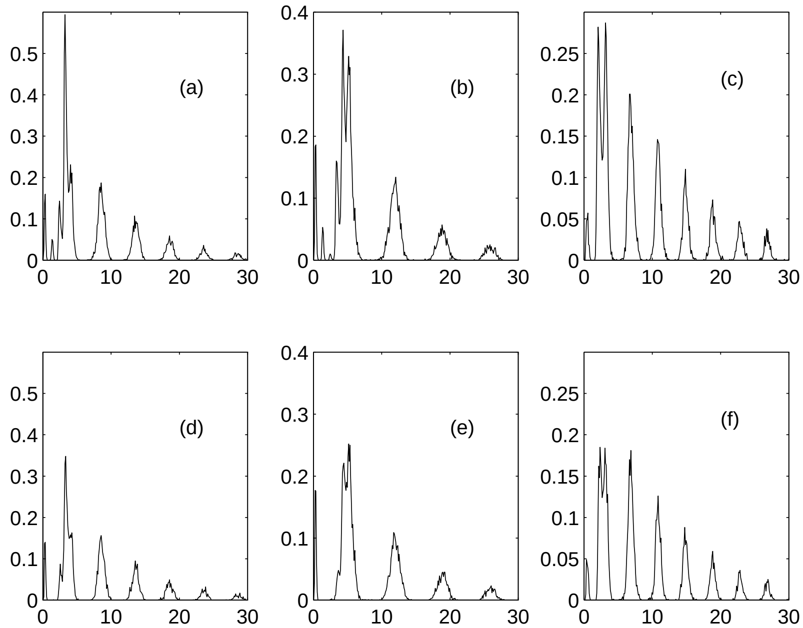

Figure 1: For $P \equiv (2\pi/\alpha) = 2, \beta = 0.1, A = 1$ and $Q = 5$ densities $g_s(t|x_0)$ and $g^+(t|x_0)$ are plotted respectively in (a) and in (d). For $P = 2, \beta = 0.1, A = 1$ and $Q = 7$ densities $g_s(t|x_0)$ and $g^+(t|x_0)$ are plotted respectively in (b) and in (e). For $P = 3, \beta = 0.1, A = 2$ and $Q = 4$ densities $g_s(t|x_0)$ and $g^+(t|x_0)$ are plotted respectively in (c) and in (f).

the $\varepsilon-$upcrossing FPT pdf $g_u^{(\varepsilon)}[S(t),t]$ related to the conditioned FPT pdf $g[S(t),t|x_0]$ as follows:

$$g_u^{(\varepsilon)}[S(t),t] = \int_{-\infty}^{S(0)-\varepsilon} g[S(t),t|x_0]\,\gamma_\varepsilon(x_0)\,dx_0, \qquad (t \geq 0),$$

under the hypothesis that a subset of sample paths of $X(t)$ are originated at a state X_0 that is a r.v. with pre-assigned pdf

$$\gamma_\varepsilon(x_0) \equiv \begin{cases} f_1(x_0)\,\left[\int_{-\infty}^{S(0)-\varepsilon} f_1(z)\,dz\right]^{-1}, & x_0 < S(0)-\varepsilon \\ 0, & x_0 \geq S(0)-\varepsilon, \end{cases} \tag{9}$$

and where $f_1(x_0)$ denotes the pdf of $X(0)$:

$$f_1(x_0) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x_0^2}{2}\right).$$

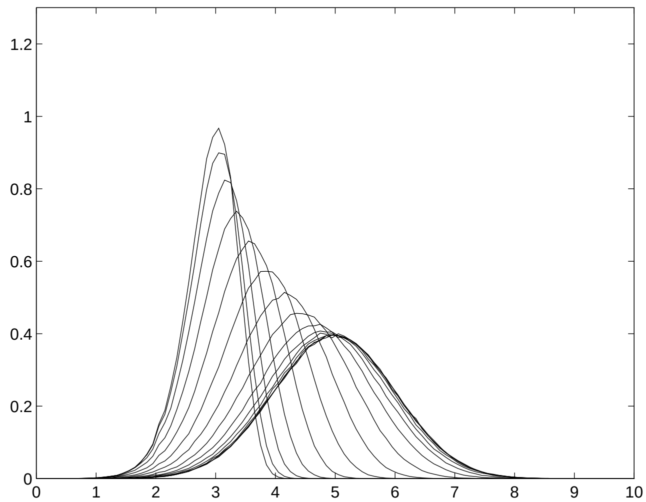

Figure 2: Plot of $g_u[S(t), t]$ for the various values of θ.

By using the parallel procedure, suitably modified ([2]) for upcrossing FPT problem, estimates of the upcrossing probability density function of the first passage time $\tilde{g}_u^{(\varepsilon)}[S(t), t]$ have been constructed. In the context of upcrossing FPT problem we also worked out a numerical procedure to evaluate $W_1^{(u)}(t)$, that plays the analogous role of $W_1(t|x_0)$ in the conditional FPT problem. A comparison is then provided with the numerical results obtained by approximating the simulated upcrossing probability density by the first order partial sum of the series expansion (see Fig.3).

3 Asymptotic results

Finally, by making use of a Rice-like series expansion, we have investigated the asymptotic behavior of FPT pdf through certain time-varying boundaries, including periodic boundaries. In [2] we gave sufficient conditions for the case of a single asymptotically constant boundary, under which the FPT densities asymptotically exhibit exponential behaviors. The parallel procedure to simulate the sample paths allows to evaluate the order of magnitude of the parameters characterizing the exponential behavior of FPT pdf's (see Fig.4).

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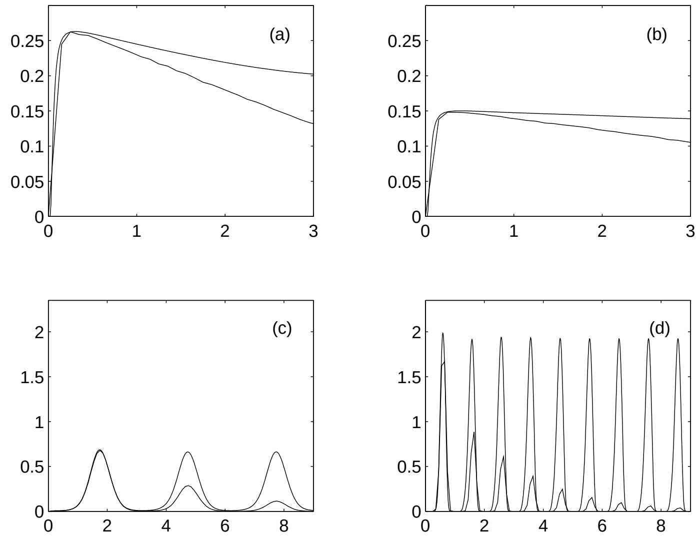

Figure 3: Plot of $W_1^{(u)}(t)$ and of $\tilde{g}_u^{(\varepsilon)}[S(t),t]$ as function of t (top to bottom) for a stationary Gaussian process with zero mean and covariance function (3) for the boundary (4) with the following parameter values: (a) $S_0 = 0.5$, $A = 0$, $\alpha = 1$ and $\varepsilon = 0.1$; (b) $S_0 = 1$, $A = 0$, $\alpha = 1$ and $\varepsilon = 0.1$; (c) $S_0 = 1$, $A = 1$, $Q = 3$, $\alpha = 1$, $\varepsilon = 0.1$; (d) $S_0 = 1$, $A = 1$, $Q = 1$, $\alpha = 1$, $\varepsilon = 0.1$.

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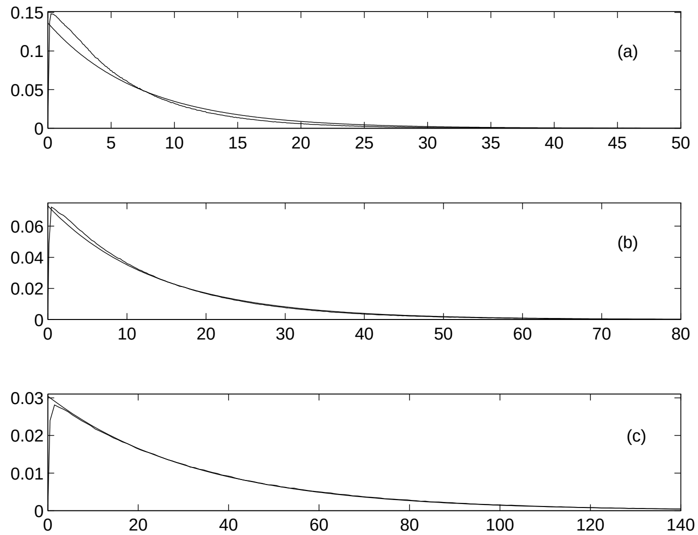

Figure 4: Plot of $\tilde{g}_u^{(\varepsilon)}(S,t)$ with $\varepsilon = 0.1$ and exponential pdf $g(t) = \lambda e^{-\lambda t}$ where λ is specified in [2], related to a Butterworth covariance function with $\alpha = 1$ and constant boundaries $S = 1$ in (a), $S = 1.5$ in (b) and $S = 2$ in (c).

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